Furan. 2-ethynyl

Inchi:	InChI=1S/C6H4O/c1-2-6-4-3-5-7-6/h1,3-5H
InchiKey:	CTVCBOZMKFQEAP-UHFFFAOYSA-N
Formula:	C6H4O
SMILES:	C#Cc1ccco1
Mol. weight [g/mol]:	92.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	1.261		Crippen Method
mcvol	73.210	ml/mol	McGowan Method
rinpol	742.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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